SEVERAL TRAJECTORY OPTIMIZATION TECHNIQUES
Part I: Discussion

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SEVERAL TRAJECTORY OPTIMIZATION TECHNIQUES

Part I: D[illegible]

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Abstract

This paper discusses several numerical approaches for solving problems arising in optimizing trajectories. The basic concepts underlying the gradient method, the second variation method, and a generalized Newton-Raphson method are presented in a very elementary manner by considering an ordinary minimum problem with a side constraint. The results obtained when the basic concepts are extended to the variational problem and the computational algorithms are then discussed. Finally, in the concluding remarks, advantages and disadvantages of each method are reviewed, and a comparison is made between the second variation method, which might be considered a direct method, and the generalized Newton-Raphson method, normally considered as an indirect method. Part II of this paper provides an application of the three methods to a specific problem.

Introduction

The numerical methods for the solution of optimization problems have in the past taken two primary directions: the direct approach and the indirect approach. In the direct approach, which is usually associated with a steep descent technique, the constraining system differential equations are satisfied and an iteration made on the control signals such that each new iterate improves the function to be minimized. The indirect approach involves the development of an iterative technique for the solution of the system and Euler-Lagrange differential equations. Advantages usually associated with the steep descent techniques are that convergence does not depend upon the availability of a good initial estimate of the optimal trajectory as a starting point, and that the techniques seek out relative minima rather than merely functionals which are stationary. The main disadvantage associated with the steep descent techniques is that in many practical applications convergence slows as the optimum trajectory is approached. In contrast, the indirect methods usually exhibit good convergence as the optimal trajectory is approached if the method converges at all. However, a good initial estimate of the optimal trajectory may be needed to ensure convergence.

Part I of this paper presents a brief review of the first and second variation theory as associated with the steep descent methods. This is followed by a discussion of a generalized Newton-Raphson method as applied to the solution of the system and Euler-Lagrange equations. Finally, a comparison between the second variation method and the generalized Newton-Raphson method is made which suggests that the second variation method is equivalent to a special case of the generalized Newton-Raphson method.

Both the steep descent methods and the generalized Newton-Raphson method have been discussed in detail by the authors and others in previous papers, see (1) through (8). Here, the purpose is to review basic concepts. This can best be accomplished by considering an ordinary minimum problem with a single side constraint and then presenting the results derived in the above references when the theory is extended to the variational case.

Part II of this paper discusses the actual computational procedures using the gradient method, second variation method, and the generalized Newton-Raphson method to solve a specific problem.

Problem Formulation

The usual Mayer formulation is employed for the variational problem. Given a system of first order differential equations

$$\dot{x}_i = f_i(x_1, \ldots, x_n, y_1, \ldots, y_\ell, t) \tag{1}$$

find a solution of this system of equations which satisfies certain specified initial and terminal conditions and minimizes P, a function of the final unspecified terminal conditions and the terminal time.

$$P = P[x_{m+1_f}, \ldots, x_{n_f}, t_f] \tag{2}$$

The x variables are referred to as the state variables and the y variables as the control variables. Both the state and control variables may be subject to constraints; however, in this discussion we will deal primarily, though not exclusively, with the case where such constraints are absent.

It will be assumed for convenience that initial values of x_i are fixed at t_0

$$x_i(t_0) = \tilde{x}_{i_0} \quad , \quad i = 1, \ldots, n \tag{3}$$

as well as the first m of the terminal values

$$x_i(t_f) = \tilde{x}_{i_f} \quad , \quad i = 1, \ldots, m \tag{4}$$

The final time t_f may or may not be specified. In the gradient method it will be convenient to reformulate the problem such that all of the final state variables are open. This is done by employing a penalty function approximation:

$$P'(x_{1_f}, \ldots, x_{n_f}, t_f) = P(x_{m+1_f}, \ldots, x_{n_f}, t_f) + \tfrac{1}{2} \sum_{j=1}^{m} K_j^2 (x_{j_f} - \tilde{x}_{j_f})^2 \tag{5}$$

A minimum of P' is now sought without requiring the terminal values of the first m state variables to satisfy Eq. (4) exactly but rather paying a "penalty" for deviations. As the K_j becomes large the trajectory which minimizes P' is in some sense close to the trajectory which minimizes P with the final values of the first m state variables specified.

At this point it is advisable to digress from the variational problem and examine an ordinary minimum problem with a subsidiary constraint. Let us consider the problem of minimizing a function of two variables constrained such that a second function of the variables is equal to zero.

$$\text{Min } f(x_1, x_2) \quad \text{subject to} \quad g(x_1, x_2) = 0 \tag{6}$$

We further assume that both f and g and their first and second partial derivatives exist for all finite values of x_1 and x_2. Expanding both f and g in a Taylor series and retaining all terms up to and including second order gives:

$$\begin{aligned} f(x_1, x_2) &= \bar{f}(\bar{x}_1, \bar{x}_2) + \bar{f}_{x_1}\Delta x_1 + \bar{f}_{x_2}\Delta x_2 \\ &\quad + \tfrac{1}{2}\bar{f}_{x_1x_1}\Delta x_1^2 + \bar{f}_{x_1x_2}\Delta x_1\Delta x_2 + \tfrac{1}{2}\bar{f}_{x_2x_2}\Delta x_2^2 \end{aligned} \tag{7a}$$

$$\begin{aligned} g(x_1, x_2) &= \bar{g}(\bar{x}_1, \bar{x}_2) + \bar{g}_{x_1}\Delta x_1 + \bar{g}_{x_2}\Delta x_2 \\ &\quad + \tfrac{1}{2}\bar{g}_{x_1x_1}\Delta x_1^2 + \bar{g}_{x_1x_2}\Delta x_1\Delta x_2 + \tfrac{1}{2}\bar{g}_{x_2x_2}\Delta x_2^2 = 0 \end{aligned} \tag{7b}$$

where the barred functions are evaluated at a specific value of x_1 and x_2. We choose $\bar{x}_1$ and $\bar{x}_2$ such that the constraint $\bar{g}(\bar{x}_1, \bar{x}_2) = 0$ is satisfied and solve for Δx_1 in terms of Δx_2 retaining first and second order terms.

$$\begin{aligned} \Delta x_1 = -\frac{1}{\bar{g}_{x_1}}\Bigg[&\bar{g}_{x_2}\Delta x_2 + \tfrac{1}{2}\bar{g}_{x_1x_1}\left(-\frac{\bar{g}_{x_2}}{\bar{g}_{x_1}}\right)^2\Delta x_2^2 \\ &+ \bar{g}_{x_1x_2}\left(-\frac{\bar{g}_{x_2}}{\bar{g}_{x_1}}\right)\Delta x_2^2 + \tfrac{1}{2}\bar{g}_{x_2x_2}\Delta x_2^2 \Bigg] \end{aligned} \tag{8}$$

It is tacitly assumed that $\bar{g}_{x_1} \neq 0$. An expression for the change in f is then obtained by substituting Eq. (8) into Eq. (7a).

$$
\begin{aligned}
f(x_1, x_2) - \bar{f}(\bar{x}_1, \bar{x}_2) = {} & \left(\bar{f}_{x_2} - \frac{\bar{f}_{x_1}}{\bar{g}_{x_1}} \bar{g}_{x_2}\right) \Delta x_2 \\
& + \tfrac{1}{2}\left(\bar{f}_{x_1 x_1} - \frac{\bar{f}_{x_1}}{\bar{g}_{x_1}} \bar{g}_{x_1 x_1}\right) \frac{\bar{g}^2_{x_2}}{\bar{g}^2_{x_1}} \Delta x_2^2 \\
& - \left(\bar{f}_{x_1 x_2} - \frac{\bar{f}_{x_1}}{\bar{g}_{x_1}} \bar{g}_{x_1 x_2}\right) \frac{\bar{g}_{x_2}}{\bar{g}_{x_1}} \Delta x_2^2 \\
& + \tfrac{1}{2}\left(\bar{f}_{x_2 x_2} - \frac{\bar{f}_{x_1}}{\bar{g}_{x_1}} \bar{g}_{x_2 x_2}\right) \Delta x_2^2
\end{aligned} \tag{9}
$$

Therefore, sufficient conditions for $\bar{f}(\bar{x}_1, \bar{x}_2)$ to be a minimum of $f(x_1, x_2)$ subject to $g(x_1, x_2)$ equal to zero are

(i) $$\bar{f}_{x_2} - \frac{\bar{f}_{x_1}}{\bar{g}_{x_1}} \bar{g}_{x_2} = 0 \quad , \quad \bar{g}_{x_1} \neq 0$$

(ii) $$
\begin{aligned}
& \tfrac{1}{2}\left(\bar{f}_{x_1 x_1} - \frac{\bar{f}_{x_1}}{\bar{g}_{x_1}} \bar{g}_{x_1 x_1}\right) \frac{\bar{g}^2_{x_2}}{\bar{g}^2_{x_1}} - \left(\bar{f}_{x_1 x_2} - \frac{\bar{f}_{x_1}}{\bar{g}_{x_1}} \bar{g}_{x_1 x_2}\right) \frac{\bar{g}_{x_2}}{\bar{g}_{x_1}} \\
& + \tfrac{1}{2}\left(\bar{f}_{x_2 x_2} - \frac{\bar{f}_{x_1}}{\bar{g}_{x_1}} \bar{g}_{x_2 x_2}\right) > 0
\end{aligned} \tag{10}
$$

Of course the conditions are symmetric with x_1 replaced with x_2 and x_2 replaced with x_1.

In the classical theory, the constraint $g(x_1, x_2) = 0$ is adjoined to $f(x_1, x_2)$ by means of a Lagrange multiplier

$$S(x_1, x_2, \lambda) = f(x_1, x_2) + \lambda g(x_1, x_2) \tag{11}$$

and S is expanded in the neighborhood of some point $\bar{x}_1$, $\bar{x}_2$, and $\bar{\lambda}$ considering all variables to have independent variations.

$$\begin{aligned} S(x_1, x_2, \lambda) &= \bar{S}(\bar{x}_1, \bar{x}_2, \bar{\lambda}) + \bar{S}_{x_1}\Delta x_1 + \bar{S}_{x_2}\Delta x_2 + \bar{g}\Delta\lambda \\ &+ \tfrac{1}{2}\bar{S}_{x_1x_1}\Delta x_1^2 + \bar{S}_{x_1x_2}\Delta x_1\Delta x_2 + \tfrac{1}{2}\bar{S}_{x_2x_2}\Delta x_2^2 \\ &+ (\bar{g}_{x_1}\Delta x_1 + \bar{g}_{x_2}\Delta x_2)\Delta\lambda \end{aligned} \tag{12}$$

Sufficient conditions for $\bar{S}(\bar{x}_1, \bar{x}_2, \bar{\lambda})$ to be a minimum of $S(x_1, x_2, \lambda)$ subject to $g(x_1, x_2)$ equal to zero are

$$\begin{aligned} &\text{(i)} && \bar{S}_{x_1} = \bar{f}_{x_1} + \bar{\lambda}\bar{g}_{x_1} = 0 \\ &\text{(ii)} && \bar{S}_{x_2} = \bar{f}_{x_2} + \bar{\lambda}\bar{g}_{x_2} = 0 \\ &\text{(iii)} && \bar{g}_{x_1}\Delta x_1 + \bar{g}_{x_2}\Delta x_2 = 0 \\ &\text{(iv)} && \tfrac{1}{2}\left(\bar{f}_{x_1x_1} + \bar{\lambda}\bar{g}_{x_1x_1}\right)\Delta x_1^2 + \left(\bar{f}_{x_1x_2} + \bar{\lambda}\bar{g}_{x_1x_2}\right)\Delta x_1\Delta x_2 \\ &&& + \tfrac{1}{2}\left(\bar{f}_{x_2x_2} + \bar{\lambda}\bar{g}_{x_2x_2}\right)\Delta x_2^2 > 0 \end{aligned} \tag{13}$$

These conditions are exactly equivalent to the sufficient conditions given in Eqs. (10i) and (10ii). Furthermore, it should be emphasized that S is merely stationary with respect to x_1, x_2, and λ and a minimum only when $g(x_1, x_2)$ is constrained to be equal to zero.

Gradient Techniques

The basis of the steep descent or gradient techniques is to search out the stationary value of S by an effective numerical iteration method. To complete the analogy between the ordinary minimum problem and the Mayer formulation of the variational problem either x_1 or x_2 is chosen as a control variable. Although Eq. (12) was used to determine the sufficient conditions for $\bar{f}(\bar{x}_1, \bar{x}_2)$ to be a minimum with $\bar{g}(\bar{x}_1, \bar{x}_2) = 0$, the expansion is valid for any value $\bar{x}_1$, $\bar{x}_2$, and $\bar{\lambda}$ and need not be at a stationary point of S.

In the gradient method initial estimates of x_1, x_2, and λ would be made that satisfy $g(x_1, x_2) = 0$ and Δx_1, Δx_2, and $\Delta\lambda$ determined from first order terms in Eq. (12) such that ΔS would decrease. Although usually one would not likely use a gradient method to solve an ordinary minimum problem of the type discussed, we will indicate how the computational algorithm might proceed so that we may see the analogy with the variational problem.

Let us assume that x_2 plays the role of the control variable. An initial guess is chosen for x_1, x_2, and λ such that $g(x_1, x_2) = 0$ and $S_{x_1} = 0$. This guess will be designated by the barred quantities in Eq. (12). We can then be sure that ΔS is negative if Δx_2 and $\bar{S}_{x_2}$ are of opposite sign.

$$\Delta S = S(x_1, x_2, \lambda) - \bar{S}(\bar{x}_1, \bar{x}_2, \bar{\lambda}) = \bar{S}_{x_2} \Delta x_2 \tag{14}$$

However, the magnitude of Δx_2 must be small enough to assure that the first order theory is valid. One could view the problem as one of minimizing ΔS subject to a constraint on the magnitude of Δx_2 if the constraint were known.

$$S' = \Delta S + \gamma(\Delta x_2^2 - K^2) = \bar{S}_{x_2} \Delta x_2 + \gamma(\Delta x_2^2 - K^2) \tag{15}$$

Here, γ acts as another Lagrange multiplier for a constrained auxiliary minimum problem. Solving for the stationary values of S' gives

$$\Delta x_2 = - \frac{\bar{S}_{x_2}}{2\gamma} \tag{16}$$

The magnitude of Δx_2 is still not determined, for γ is unspecified. A one dimensional search is normally made varying γ and calculating $S(x_1, x_2)$. In this simple problem one could just as well have performed the one dimensional search directly on Δx_2, however, in an n dimensional problem Eqs. (15) and (16) become

$$S' = \sum_{i=2}^{n} S_{x_i} \Delta x_i + \gamma \left(\sum_{i=2}^{n} \Delta x_i^2 - K^2 \right) \tag{17}$$

$$\Delta x_i = - \frac{\bar{S}_{x_i}}{2\gamma} \quad , \qquad i = 2, \ldots, n \tag{18}$$

For the n dimensional problem we can appreciate how the gradient method received its name. If we consider the x_i, $i = 2, \ldots, n$ components of an $n-1$ vector, the $\vec{\Delta x}$ vector is in the negative gradient direction of S.

These concepts as applied to the variational problem have been discussed in detail in (1) through (4), and therefore, only the results are summarized here. The Lagrange multipliers become functions of time which obey the system of differential equations

$$\dot{\lambda}_i = - \sum_{j=1}^{n} \lambda_j \frac{\partial f_j}{\partial x_i} \quad , \quad \lambda_i(\bar{t}_f) = \frac{\partial P'}{\partial x_i} \quad , \quad i = 1, \ldots, n \tag{19}$$

For convenience the function $H(\vec{x}, \vec{\lambda}, \vec{y}, t)$ is defined:

$$H(\vec{x}, \vec{\lambda}, \vec{y}, t) = \sum_{i=1}^{n} \lambda_i f_i (\vec{x}, \vec{y}, t) \tag{20}$$

where

$$\begin{aligned} \vec{x}^T &\equiv x_1, \ldots, x_n \\ \vec{\lambda}^T &\equiv \lambda_1, \ldots, \lambda_n \\ \vec{y}^T &\equiv y_1, \ldots, y_\ell \end{aligned} \tag{21}$$

The superscript denotes the transpose of the vector. Equations (1) and (19) can then be put in a canonical form:

$$\begin{aligned} \dot{x}_i &= \frac{\partial H}{\partial \lambda_i}, \quad x_i(t_0) = \tilde{x}_{i_0} \\ \dot{\lambda}_i &= -\frac{\partial H}{\partial x_i}, \quad \lambda_i(t_f) = \frac{\partial P'}{\partial x_i} \end{aligned} \tag{22}$$

From first order theory we may write an equation for $P'(\vec{x}_f, t_f)$

$$\begin{aligned} P'(\vec{x}_f, t_f) &= \bar{P}'(\vec{\bar{x}}_f, \bar{t}_f) + \int_{t_0}^{t_f} \frac{\partial H}{\partial y_k} \delta y_k \, dt \\ &+ \left[\frac{\partial \bar{P}'}{\partial x_{i_f}} \bar{f}_i(\vec{\bar{x}}, \vec{\bar{y}}, \bar{t}_f) + \frac{\partial \bar{P}'}{\partial t_f} \right] \delta t_f \end{aligned} \tag{23}$$

Necessary conditions for $\bar{x}(t)$ to be an optimum trajectory and $\bar{y}(t)$ the optimum control are

$$\frac{\partial \bar{H}}{\partial y_k} = 0 \tag{24}$$

and if final time is open

$$\left.\frac{d\bar{P}'}{dt}\right|_{t=\bar{t}_f} = \frac{\partial \bar{P}'}{\partial x_{i_f}} \bar{f}_i(\vec{\bar{x}}, \vec{\bar{y}}, \bar{t}_f) + \frac{\partial \bar{P}'}{\partial t_f} = 0 \tag{25}$$

In addition, of course, $\bar{x}$ and $\bar{\lambda}$ must satisfy Eq. (22).

As in the case of the ordinary minimum problem the barred variables in Eq. (22) need not be optimum trajectories. Therefore if $\vec{\bar{x}}$ is a nonoptimum trajectory, the gradient method provides an effective numerical iteration technique for choosing a $\vec{\delta y}$ vector to decrease the value of $P'(\vec{x}_f, t_f)$. Just as in the ordinary minimum problem we now consider an auxiliary minimum problem with a constraint on $\vec{\delta y}$ adjoined to ensure that the first order theory remains valid

$$\Delta P^{*'} = P'(\vec{x}_f, t_f) - P'(\vec{\bar{x}}_f, \bar{t}_f) + \sum_{k=1}^{\ell} \gamma_k \left\{ \int_{t_0}^{\bar{t}_f} w_k(t)\, \delta y_k^2 \, dt - a_k^2 \right\} \tag{26}$$

where $w_k(t)$ is a weighting function which in many cases is given the value of unity. A constraint could also be imposed on δt_f; however, in practice the determination of δt_f can best be accomplished in a different manner which will be explained when the actual computational procedure is discussed. The solution of the auxiliary minimum problem leads to an equation for $\vec{\delta y}$ as a function of time

$$\delta y_k = - \frac{1}{c_k w_k(t)} \frac{\partial \bar{H}}{\partial y_k} \tag{27}$$

As in the ordinary minimum problem the undetermined constants c_k appear and are found by an independent search procedure. For example, if there is only one control variable, P' would be calculated for several values of c and then a polynomial fit made to determine the value of c which gives the least value to P'.

The actual computer algorithm might proceed as follows:

1. Select an initial control time history as a first estimate and numerically integrate the system equations (1).

2. Terminate the trajectory calculations at the time $\bar{t}_f$ determined when P' reaches a minimum.
3. Integrate the adjoint system backwards using terminal values determined by $\lambda_i(\bar{t}_f) = \frac{\partial P'}{\partial x_{i_f}}$.

   During the backwards integration calculate $\delta y_k(t) = -\frac{1}{c_k w_k(t)} \frac{\partial H}{\partial y_k}$.
4. Integrate the system equations forward with $y_k = \bar{y}_k + \delta y_k$ for several values of c_k and evaluate $P'(\vec{x}_f, t_f)$ again terminating the trajectory when $\frac{dP'}{dt_f} = 0$.
5. Using a curve fitting technique find the best values for c_k and use this value to determine the next estimate for y_k: $y_k = \bar{y}_k + \delta y_k$. Return to step 1 and repeat.

This procedure has proved quite successful in the past. Several variations of the method are also used extensively. If constraints are imposed on the control variables a more general expression derived from the Pontryagin Maximum Principle, (9) and (10), is used for P' in place of Eq. (23).

$$P'(\vec{x}_f, t_f) = \bar{P}'(\vec{\bar{x}}_f, \bar{t}_f)$$

$$+ \int_{t_0}^{t_f} \left\{ H(\vec{\bar{x}}, \vec{\bar{\lambda}}, \vec{\bar{y}} + \vec{\delta y}, t) - H(\vec{\bar{x}}, \vec{\bar{\lambda}}, \vec{\bar{y}}, t) \right\} dt$$

$$+ \left\{ \bar{H}(\vec{\bar{x}}_f, \vec{\bar{\lambda}}_f, \vec{\bar{y}}_f, \bar{t}_f) + \frac{\partial \bar{P}'}{\partial t} \right\} \delta t_f \tag{28}$$

Equation (27) is then replaced with the criterion that $H(\vec{\bar{x}}, \vec{\bar{\lambda}}, \vec{\bar{y}} + \vec{\delta y}, t) + \sum_{k=1}^{\ell} \gamma_k \delta y_k^2$ be a minimum within the admissible range of the control variables.

Although a quadratic constraint was used to assure that the new trajectory was neighboring to the estimated trajectory, many other constraints could also be used. One that is particularly useful when the optimum control is "bang-bang" or on-off is an integral absolute value constraint. In this case Eq. (27) is replaced with the criterion that $H(\vec{\bar{x}}, \vec{\bar{\lambda}}, \vec{\bar{y}} + \delta\vec{y}, t) + \sum_{k=1}^{\ell} \gamma_k |\delta y_k|$ be a minimum while satisfying the constraints on the control variables, $\vec{y} = \vec{\bar{y}} + \delta\vec{y}$. It is easily seen that when the control variable δy_k appears linearly in H that every intermediate control estimate will be "bang-bang" or on-off. (The singular case is excluded where the coefficient y_k in H is identically zero over a finite interval of time.) The constants γ_k are determined by an independent search as before.

Another variation of the gradient method is discussed in (3) and referred to as the Min H method. Here $H(\vec{\bar{x}}, \vec{\bar{\lambda}}, \vec{\bar{y}} + \delta\vec{y}, t)$ is minimized by the choice of $\delta\vec{y}$ satisfying any constraints that might be imposed on $\vec{y}$. In place of the rather arbitrary absolute value and quadratic metrics previously used to ensure neighboring trajectories we set

$$y_k = \bar{y}_k + \alpha_k \delta y_k \tag{29}$$

and an independent search is made as before to determine α_k.

When constraints on the state variables are present some success has been experienced (11) when additional penalty function terms are added to the function to be minimized:

$$P'' = P' + \sum \beta_j \int_{t_0}^{t_f} U_{-1}[g_j(\vec{x}, t)]dt \tag{30}$$

where U_{-1} is the Heaviside step function and $g_j(\vec{x}, t) \leq 0$ the state constraints. The constants β_j are allowed to approach infinity as in the case when penalty function terms are used in place of satisfying terminal end conditions.

The principal advantage of the gradient method is that convergence is not contingent upon a good initial estimate of the trajectory. One is assured that the value of the function to be minimized is decreased in each succeeding iteration. There are three principal disadvantages of the method. First, the convergence, although usually relatively good in the beginning of the iterative sequence, often deteriorates severely as the optimum trajectory is approached. Second, the penalty function method required to solve problems with specified terminal conditions introduces arbitrary constants which are required to be "large" (certainly a relative measure) at least for the final iteration. If the constants are chosen too large at any point in the iteration cycle, the new control will tend to improve the specified terminal values without much weight being placed on improving the actual function to be minimized. If the constants are too small the specified terminal values will not be satisfied. Thus in practice, the success of the method depends to an appreciable extent upon past experience in making proper choices for the arbitrary constants associated with the penalty function terms. Third, regions of severe irregularity sometimes develop in the control variable functions. In extreme cases these are never smoothed out.

Second Variation Method

A natural extension of the gradient techniques which come from first order theory is a theory which would include second order terms in the expression for the function to be minimized. Let us return to the ordinary minimum problem and the expression for $S(x_1, x_2, \lambda)$ given in Eq. (12). Assuming, as before, that $\bar{x}_1$ and $\bar{x}_2$ satisfy $\bar{g} = 0$ we treat the auxiliary problem of finding the stationary value of S considering Δx_1, Δx_2, and $\Delta\lambda$ as independent variables:

$$\begin{aligned} \bar{S}_{x_1} + \bar{S}_{x_1x_1}\Delta x_1 + \bar{S}_{x_1x_2}\Delta x_2 + \bar{g}_{x_1}\Delta\lambda &= 0 \\ \bar{S}_{x_2} + \bar{S}_{x_1x_2}\Delta x_1 + \bar{S}_{x_2x_2}\Delta x_2 + \bar{g}_{x_2}\Delta\lambda &= 0 \\ \bar{g}_{x_1}\Delta x_1 + \bar{g}_{x_2}\Delta x_2 &= 0 \end{aligned} \tag{31}$$

One could also view the problem as that of finding the minimum of $S(x_1, x_2, \lambda)$ considering λ fixed and a constraint adjoined which requires $\bar{g}_{x_1} \Delta x_1 + \bar{g}_{x_2} \Delta x_2 = 0$. In this case the $\Delta\lambda$ would be viewed as another Lagrange multiplier. A step size constraint may also be required as in the first order theory to ensure that the second order theory is valid. Then in Eq. (31)

$$\begin{aligned} \bar{S}_{x_1x_1} &\to \bar{S}_{x_1x_1} + \gamma \\ \bar{S}_{x_2x_2} &\to \bar{S}_{x_2x_2} + \gamma \end{aligned} \tag{32}$$

It should be noted that Eq. (31) is a linearization of Eqs. (13i) and (13ii) and the constraint equation $g(x_1, x_2) = 0$.

In the variational problem we will first consider the case for which the penalty function technique is used in place of satisfying terminal conditions exactly. The penalty function terms will then be removed and the terminal conditions satisfied exactly. The actual derivation of the equations is quite involved and therefore we summarize the results derived in (5).

$$\delta\dot{x}_i = \sum_{j=1}^{n} \frac{\partial^2 \bar{H}}{\partial\lambda_i \partial x_j}\,\delta x_j + \sum_{k=1}^{\ell} \frac{\partial^2 \bar{H}}{\partial\lambda_i \partial y_k}\,\delta y_k \quad , \tag{33a}$$

$$\delta x_i(0) = 0$$

$$\begin{aligned} \delta\dot{\lambda}_i = &- \sum_{j=1}^{n} \frac{\partial^2 \bar{H}}{\partial x_i \partial x_j}\,\delta x_j - \sum_{k=1}^{\ell} \frac{\partial^2 \bar{H}}{\partial x_i \partial y_k}\,\delta y_k \\ &- \sum_{j=1}^{n} \frac{\partial^2 \bar{H}}{\partial x_i \partial \lambda_j}\,\delta\lambda_j \end{aligned} \tag{33b}$$

$$\Delta\lambda_i(\bar{t}_f) = \sum_{j=1}^{n} \frac{\partial^2 \bar{P}'}{\partial x_{j_f} \partial x_{i_f}} \Delta x_j(\bar{t}_f) + \frac{\partial^2 \bar{P}'_i}{\partial t_f \partial x_{i_f}} \delta t_f \tag{33c}$$

$$\Delta x_i(\bar{t}_f) = \delta x_i(\bar{t}_f) + \dot{\bar{x}}_i(t_f)\delta t_f \tag{33d}$$

$$\Delta\lambda_i(\bar{t}_f) = \delta\lambda_i(\bar{t}_f) + \dot{\bar{\lambda}}_i(t_f)\delta t_f \qquad i = 1, \ldots, n \tag{33e}$$

$$\begin{aligned} &\frac{\partial \bar{H}}{\partial y_k} + \sum_{j=1}^{n} \frac{\partial^2 \bar{H}}{\partial y_k \partial x_j} \delta x_j + \sum_{j=1}^{n} \frac{\partial^2 \bar{H}}{\partial y_k \partial \lambda_j} \delta\lambda_j \\ &\quad + \sum_{s=1}^{\ell} \frac{\partial^2 \bar{H}}{\partial y_k \partial y_s} \delta y_s = 0 \qquad k = 1, \ldots, \ell \end{aligned} \tag{33f}$$

and the following equation evaluated at $\bar{t}_f$

$$\begin{aligned} &\sum_{i=1}^{n} \frac{\partial \bar{P}}{\partial x_{i_f}} \bar{f}_i + \frac{\partial \bar{P}}{\partial t_f} + \sum_{i,j=1}^{n} \frac{\partial^2 \bar{P}}{\partial x_{i_f} \partial x_{j_f}} \bar{f}_i \Delta x_j(\bar{t}_f) \\ &+ \sum_{i,j=1}^{n} \frac{\partial \bar{P}}{\partial x_{i_f}} \frac{\partial \bar{f}_i}{\partial x_{j_f}} \Delta x_j(\bar{t}_f) + \sum_{k=1}^{\ell} \sum_{i=1}^{n} \frac{\partial \bar{P}}{\partial x_{i_f}} \frac{\partial \bar{f}_i}{\partial y_{k_f}} \Delta y_k(\bar{t}_f) \\ &+ \sum_{i=1}^{n} \frac{\partial \bar{P}}{\partial x_{i_f}} \frac{\partial \bar{f}_i}{\partial t_f} \delta t_f + \sum_{i=1}^{n} \frac{\partial^2 \bar{P}}{\partial x_{i_f} \partial t_f} f_i \delta t_f \\ &+ \sum_{i=1}^{n} \frac{\partial^2 \bar{P}}{\partial x_{i_f} \partial t_f} \Delta x_i(\bar{t}_f) + \frac{\partial^2 P}{\partial t_p^2} \delta t_f = 0 \end{aligned} \tag{33g}$$

where

$$\Delta y_k(\bar{t}_f) = \delta y_k + \dot{\bar{y}}_k \delta t_f$$

These equations, as we might have anticipated from the analysis of the ordinary minimum problem, are a linearization of the necessary condition for a minimum as derived from the first order theory. Again, an integral step size constraint may be required for $\vec{\delta y}$ in which event the diagonal terms of the array $(\partial^2 H)/(\partial y_k \partial y_s)$ would have positive constants added to them.

The actual computational procedure might proceed as follows:

1. Select an initial control time history as a first estimate and numerically integrate the system equations (1) as in the gradient method. Terminate the calculation at time $\bar{t}_f$ determined such that $(dP')/(dt_f) = 0$.
2. Integrate the adjoint system backwards using terminal values determined by $\lambda_i(\bar{t}_f) = (\partial P')/(\partial x_{i_f})$ and store the initial values of $\lambda_i(t_0)$.
3. Generate a partitioned transition matrix for the linearized system and linearized adjoint system by n simultaneous integrations of linearized systems with one of the $\delta\lambda_i(0)$ equal to 1 and the remaining $\delta\lambda(0)$ equal to zero for each integration. The $\delta x_i(0)$ are all equal to zero. The homogeneous part of the control law as obtained from Eq. (33f) is substituted in the linearized systems equations for the calculation of the partitioned transition matrix.
4. The linearized system and adjoint system are integrated once again for the inhomogeneous part of the solution due to the term $(\partial\bar{H})/(\partial y_k)$ in the control law. For this integration all the $\delta\lambda_i(0)$ are equal to zero.
5. By linear algebraic operations the $\delta\lambda_i(t_0)$ are determined so as to satisfy Eqs. (33c), (33d), (33e), and (33g).
6. Another integration of the combined systems is performed with these values of $\delta\lambda_i(t_0)$ and

δy_k calculated and added to $\bar{y}_k$. Return to step 1 and repeat the process.

The process continues until the decrements in P' become small. The penalty function technique is then dropped in preference to satisfying terminal conditions exactly. Equations (33) are modified appropriately. The $\Delta x_i(\bar{t}_f)$ for the first m state variables are chosen to make $x_i(\bar{t}_f + \delta t)$ equal to $\tilde{x}_{i_f}$.

$$\Delta x_i(\bar{t}_f) = \tilde{x}_{i_f} - \bar{x}_i(\bar{t}_f) \quad , \quad i = 1, \ldots, m \tag{34}$$

Equation (33c) remains the same for $i = m+1, \ldots, n$. Of course the appropriate summation indices are changed throughout Eq. (33) to be consistent with the payoff P (the prime is dropped) being only a function of last $n-m$ state variables and final time.

The computational procedure is quite similar to the procedure sketched earlier when the penalty function technique was used. The adjoint system is integrated numerically forward with initial values $\bar{\lambda}_{i_0} + \delta\lambda_{i_0}$, $i = 1, \ldots, n$ of the preceding cycle. The modified terminal conditions of the linearized system and adjoint system are satisfied using linear algebraic procedures as before.

One advantage of the second variation method is that in the final stages of the computational procedure the penalty function technique is no longer needed and each successive approximation attempts to satisfy the boundary conditions exactly. Thus the undetermined constants associated with the penalty function terms are eliminated. A second advantage is that in both phases (penalty function and nonpenalty functions) the step size is automatically determined thus eliminating the independent search procedure needed in the gradient methods. In addition to the two main advantages listed above, most of the information necessary to perform the generalized Jacobi test is available. Also, the matrix elements for the second variational guidance scheme discussed in (12) are available as an end result of the computational process.

The disadvantages of the method lie chiefly in the additional programming effort needed to formulate the computing algorithm. However, the over-all actual computing time is considerably less as discussed in (5) and

Part II of this paper. In the present state of the art, the method is applicable only to problems where the control signal is unbounded and continuous. Extensions to bounded control variables which lead to an on-off type control signal are being investigated.

Generalized Newton-Raphson Method

We will now proceed to discuss an indirect method which on the surface does not appear to be related to the steep descent techniques or variations thereof. The method couched in the framework of functional analysis is developed in (6) from an application of the Contraction Mapping Principle. In essence, it is a generalization of a Newton-Raphson method applied to the system and Euler-Lagrange equations, and contrasts sharply with the more usual indirect approach which has had such a dismal computational past. For example, in the usual procedure sets of initial conditions are successively mapped into new sets of initial conditions and the differential constraints satisfied whereas in the generalized Newton-Raphson technique a mapping is produced which transforms sets of functions into improved sets of functions which do not necessarily satisfy the differential constraints and thus, as one might expect, yields a greater tenacity of convergence.

Let us again consider the ordinary minimum problem with a single constraint. The Euler-Lagrange equations (13i) and (13ii) and the constraint condition which is analogous to the system equations are repeated below.

$$\begin{aligned} S_{x_1} &= f_{x_1} + \lambda g_{x_1} = 0 \\ S_{x_2} &= f_{x_2} + \lambda g_{x_2} = 0 \\ S_{\lambda} &= g(x_1, x_2) = 0 \end{aligned} \tag{35}$$

A Newton-Raphson approach to the solution of these equations might proceed as follows. Select an initial x_1, x_2, and λ which need not satisfy any of the equations given in Eq. (35). Designate these values as barred variables as before and expand Eq. (35) in a Taylor series keeping only zero and first order terms

$$\bar{S}_{x_1} + \bar{S}_{x_1x_1}\Delta x_1 + \bar{S}_{x_1x_2}\Delta x_2 + \bar{g}_{x_1}\Delta\lambda = 0$$

$$\bar{S}_{x_2} + \bar{S}_{x_1x_2}\Delta x_1 + \bar{S}_{x_2x_2}\Delta x_2 + \bar{g}_{x_2}\Delta\lambda = 0 \qquad (36)$$

$$\bar{g}(x_1x_2) + \bar{g}_{x_1}\Delta x_1 + \bar{g}_{x_2}\Delta x_2 = 0$$

Equations (36) would then be solved for Δx_1, Δx_2, and $\Delta\lambda$ and new values of x_1, x_2, and λ determined.

$$x_1 = \bar{x}_1 + \Delta x_1$$

$$x_2 = \bar{x}_2 + \Delta x_2 \qquad (37)$$

$$\lambda = \bar{\lambda} + \Delta\lambda$$

The procedure continues until Eqs. (35) are satisfied or until some measure of error has decreased sufficiently.

When this technique is applied to the variational problem, the following equations result.

$$\delta\dot{x}_i = \frac{\partial\bar{H}}{\partial\lambda_i} - \dot{\bar{x}}_i + \sum_{j=1}^{n} \frac{\partial^2\bar{H}}{\partial x_i\partial x_j}\,\delta x_j + \sum_{k=1}^{\ell} \frac{\partial^2\bar{H}}{\partial\lambda_i\partial y_k}\,\delta y_k \qquad (38a)$$

$$\delta x_i(0) = 0 \quad , \quad i = 1, \ldots, n$$

$$\Delta x_i(t_f) = \tilde{x}_{i_f} - \bar{x}_{i_f} \qquad (38b)$$

$$\Delta x_i(t_f) = \delta x_i(\bar{t}_f) + \dot{\bar{x}}_i\delta t_f \quad , \quad i = 1, \ldots, m \qquad (38c)$$

$$\delta\dot{\lambda}_i = -\frac{\partial\bar{H}}{\partial x_i} - \dot{\bar{\lambda}}_i - \sum_{j=1}^{n} \frac{\partial^2\bar{H}}{\partial x_i \partial x_j}\delta x_j - \sum_{k=1}^{\ell} \frac{\partial^2\bar{H}}{\partial x_i \partial y_k}\delta y_k$$

$$- \sum_{j=1}^{n} \frac{\partial^2\bar{H}}{\partial x_i \partial\lambda_j}\delta\lambda_j \quad , \quad i = 1, \ldots, n \tag{38d}$$

$$\Delta\lambda_i(t_f) = \frac{\partial\bar{P}}{\partial x_{i_f}} - \bar{\lambda}_i(\bar{t}_f) + \sum_{j=1}^{n} \frac{\partial^2\bar{P}}{\partial x_{i_f}\, \partial x_{j_f}}\Delta x_j(\bar{t}_f)$$

$$+ \frac{\partial^2\bar{P}_i}{\partial x_{i_f}\, \partial t_f}\delta\bar{t}_f \tag{38e}$$

$$\Delta\lambda_i(t_f) = \delta\lambda_i(t_f) + \dot{\bar{\lambda}}_i\delta t_f \quad , \quad i = m+1, \ldots, n \tag{38f}$$

$$\frac{\partial\bar{H}}{\partial y_k} + \sum_{j=1}^{n} \frac{\partial^2\bar{H}}{\partial y_k \partial x_j}\delta x_j + \sum_{j=1}^{n} \frac{\partial^2\bar{H}}{\partial y_k \partial\lambda_j}\delta\lambda_j$$

$$+ \sum_{s=1}^{\ell} \frac{\partial^2\bar{H}}{\partial y_k \partial y_s}\delta y_s = 0 \quad , \quad k, \ldots, \ell \tag{38g}$$

and

$$\sum_{i=1}^{n} \frac{\partial\bar{P}}{\partial x_{i_f}}\bar{f}_i + \frac{\partial\bar{P}}{\partial t_f} + \sum_{i,j=1}^{n} \frac{\partial^2\bar{P}}{\partial x_{i_f}\, \partial x_{j_f}}\bar{f}_i \Delta x_j(\bar{t}_f)$$

$$+ \sum_{i,j=1}^{n} \frac{\partial\bar{P}}{\partial x_{i_f}} \frac{\partial\bar{f}_i}{\partial x_{j_f}}\Delta x_j(\bar{t}_f) + \sum_{k=1}^{\ell}\sum_{j=1}^{n} \frac{\partial\bar{P}}{\partial x_{i_f}} \frac{\partial\bar{f}_i}{\partial y_k}\Delta y_k(t_f) = 0 \tag{38h}$$

evaluated at $\bar{t}_f$. The penalty function technique has not been used in this formulation. It should be noted that the initial estimates for trajectories or the Lagrange multiplier time histories need not satisfy their respective differential equations.

A computational procedure might proceed as follows.

1. Analytically solve for y_k in terms of x_i, λ_i, and t and substitute the control law into the system and adjoint system equations. Select a system trajectory and ajoint trajectory that need not satisfy the differential constraints, but that does satisfy the initial conditions and perhaps, although not necessarily, the specified terminal conditions.
2. Calculate a partitioned transition matrix for the homogeneous linearized systems and adjoint system as in the second variation method by setting $\delta x_i(0) = 0$ and letting the $\delta\lambda_i(0)$ take on unity values as before.
3. Solve the system and adjoint system again for the nonhomogeneous part of the solutions.
4. Using linear algebraic relationships determine the $\delta\lambda_i(0)$ required to satisfy boundary conditions in Eqs. (38).
5. With these values for $\delta\lambda_i(0)$ integrate both linearized systems and add the $\delta\vec{x}(t)$ and $\delta\vec{\lambda}(t)$ to obtain new estimates of $\vec{x}(t)$ and $\vec{\lambda}(t)$.
6. Return to step 1 and repeat.

Because of the additional degree of freedom given by not requiring the trajectories or the adjoint system to satisfy the differential constraints there are many variations for the computational procedure. In (6) some discussion has been given to sufficient conditions for convergence using as a metric the maximum deviation between the approximate trajectory and the actual trajectory. However, in practice it has been found that the region of convergence is somewhat larger than that described by these sufficient conditions. A few examples of the numerical application of the Newton-Raphson operator technique are described in (13).

Conclusions

Several methods have been described for the numerical solution of optimization problems. The gradient technique and possibly the second variation method might be described as direct methods while the generalized

Newton-Raphson technique would no doubt be considered of the indirect type.

The advantages of the gradient method and variations of this method are in its simplicity. The convergence of the method is not contingent upon a good initial estimate as a starting condition. It is assured that the function to be minimized is decreased after each iteration cycle. There is no difficulty in handling constraints imposed on th control variables. Successful results have also been obtained when constraints were imposed on the state variables by employing an integral type penalty function. The major disadvantage of the method is in the way specified terminal conditions must be treated using penalty functions which introduce undetermined constants and often slows convergence as the optimal trajectory is approached. In addition, the step size is unspecified which also introduces additional constants which must be evaluated by independent search techniques.

Original motivation for the second variation method was to improve the iteration technique and eliminate the shortcomings of the gradient method. In the final stages of the second variation method, the penalty function technique is dropped in preference to satisfying specified terminal conditions exactly which improves convergence properties of the iterative technique as the optimal trajectory is approached. In addition, the step size is inherently determined by the method eliminating the need for evaluating undetermined constants by an independent search as is required in the gradient methods. As a by-product, the Jacobi test can be performed with little additional computation and the matrix coefficients needed for the second variation guidance are available from the final iteration cycle. The over-all saving in computer time seems to be in the order of 50 per cent, at least for the limited experience available. The disadvantages of the method are that the computer program is significantly more complicated and the method as it presently stands is not directly applicable to the case where constraints are imposed on the control signals.

The Generalized Newton-Raphson method is an indirect approach which iterates to a solution of the system and Euler-Lagrange equations which have mixed boundary conditions. An examination of the ordinary minimum problem with a single side constraint, illustrates that the significant difference between the second variation method and the generalized Newton-Raphson method is that in the former the constraint is satisfied exactly while in the latter the constraint is satisfied when the method converges to the optimum value. However, both methods systematically search out the stationary value of S. One should be able to take advantage of the additional degree of freedom available in the Newton-Raphson method to improve the computing algorithm. However, in the second variation method one can argue certain convergence properties since a minimum of the function or functional is being sought when the constraints are satisfied (at least when the penalty function is used) rather than seeking out merely stationary values of function or functional as is done in the generalized Newton-Raphson method. In summary, one might say that the generalized Newton-Raphson method is a more general form of the second variation method or conversely, the second variation method is a specific approach to the generalized Newton-Raphson method. This seems to be a common meeting ground for a direct and indirect approach to the solution of optimization problems.

As is usually the case, it is difficult to state dogmatically the superiority of any one method over another. Each method should be used where its advantages can be maximized and disadvantages minimized. A combination of two or more of the methods in practice might well be used to advantage. For example, one might initially use a gradient method or the second variation method with penalty functions to satisfy terminal constraints so as to be assured of convergence and then switch to the generalized Newton-Raphson procedure as the optimum trajectory is approached to take advantage of the possible improved rate of convergence of the latter method in the terminal phase of the iteration technique.

In Part II of this paper the application of all three methods to a specific problem will be discussed. Some of the salient features of the actual computational procedures will be brought out and a comparison made of actual computing time for the different methods.

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